Universal Crossover in Variable Range Hopping with Coulomb Interactions

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Using dimensional analysis, we show that the variable-range-hopping resistivity ρ of disordered systems with Coulomb interactions obeys the scaling form $\ln(\rho/\rho_0)=Af(T/T_x)$, where $f(x)$ is a universal function and A and T_x are sample-dependent constants. A simple heuristic calculation in three dimensions yields an explicit form for $f(x)$, which exhibits a smooth crossover from the Mott ($f\propto x^{-1/4}$) to the Efros-Shklovskii ($f\propto x^{-1/2}$) behaviors. Data on five different samples of compensated n-type CdSe are shown to collapse onto this single function.

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The variable-range-hopping (VRH) resistivity of three-dimensional disordered systems was shown by Mott [1,2] to behave as $\ln\rho\propto(T_0/T)^{1/4}$. Later, Efros and Shklovskii (ES) [3,4] argued that Coulomb interactions create a gap that leads to $\ln\rho\propto(T_0'/T)^{1/2}$ at low temperatures. Recently, some of us reported [5] the observation of a crossover with decreasing temperature from the Mott to the ES behavior in insulating n-type CdSe. In the present Letter we discuss this crossover quantitatively. We show that the resistivity data generally obey the scaling form

$$\ln(\rho/\rho_0)=Af(T/T_x)\,, \tag{1}$$

where the scale factors A and T_x depend on the individual sample properties, but the function $f(x)$ is *universal*. The function f has the limiting behaviors

$$f(x)\propto\begin{cases}x^{-1/4}, & x\gg 1,\\ x^{-1/2}, & x\ll 1,\end{cases} \tag{2}$$

yielding the Mott and ES limits. Using data taken from Ref. [5], the resistance is plotted as a function of temperature in Fig. 1 for five samples of compensated n-type CdSe containing the different net In concentrations listed in Table I. Figure 2 shows the same data scaled by the factors A and T_x listed in Table I. Note that different samples cover different ranges on the graph and all the data collapse onto a single universal curve, as predicted by Eq. (1).

In the second part of this Letter, we present a simple heuristic calculation which yields an explicit form for the crossover function,

$$f(x)=\frac{1+[(1+x)^{1/2}-1]/x}{[(1+x)^{1/2}-1]^{1/2}}\,. \tag{3}$$

The function $f(x)$ is given by the full line in Fig. 2. The excellent fit to the data for five different n-type CdSe samples leads us to believe that Eq. (3) captures the essential physics of this complicated crossover to hopping transport with Coulomb interactions.

We first give a general argument as to why a scaling of the form (1) might be expected. Both Mott and ES find that $\ln\rho\propto R_h/\xi$, where R_h is the hopping distance and ξ is the localization length. Mott finds $R_h^{M}/\xi\propto(T_0/T)^{1/4}$, and ES find $R_h^{ES}/\xi\propto(T_0'/T)^{1/2}$, with proportionality constants of order unity. Further, ES argue that hops which take advantage of the Coulomb energy may occur only for $R_h^{ES}\gg R_h^{M}$. Since both R_h^{ES} and R_h^{M} depend on T, the equation $R_h^{ES}=R_h^{M}$ identifies the *crossover temperature* [6] $T_x\propto(T_0')^2/T_0$. Since we expect the Mott behavior for $T\gg T_x$ and the ES behavior for $T\ll T_x$, it is natural to expect that both R_h and $\ln\rho$ depend on T only through the *scaled* variable T/T_x, as in Eq. (1). Assuming further the asymptotic forms of Eq. (2), we also identify $A\propto(T_0/T_0')^{1/2}$.

We next explain the derivation of Eq. (3). Both the

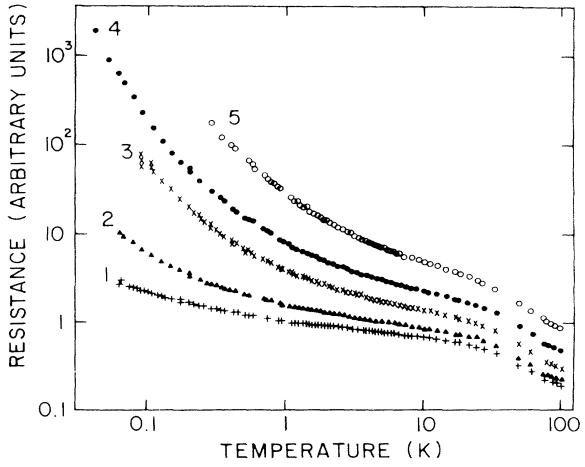

FIG. 1. Resistance vs temperature plotted on a double logarithmic scale for five insulating compensated n-type CdSe samples with net dopant concentrations listed in Table I. The data are taken from Ref. [5].

TABLE I. Sample designation, net dopant concentration N, and parameters A, T_x, T_0, and T_0' obtained from nonlinear fits of the data of Ref. [5] by Eqs. (1) and (3). Also listed for comparison are $(T_0)^I$ and $(T_0')^I$ estimated in the earlier studies [5]. The critical concentration for the metal-insulator transition is approximately 3×10^{17} cm^{-3}.

Sample	N (10^{17} cm^{-3})	A	T_x (10^{-3} K)	T_0 (K)	T_0' (K)	$(T_0)^I$ (K)	$(T_0')^I$ (K)
1	2.65	4.85 ± 0.35	0.71 ± 0.14	0.40 ± 0.14	0.076 ± 0.02	0.65	0.10
2	2.40	3.92 ± 0.20	5.5 ± 0.7	1.30 ± 0.3	0.38 ± 0.06	3.8	0.37
3	2.25	7.08 ± 0.77	6.7 ± 0.6	17.0 ± 7.5	1.50 ± 0.35	29.0	1.6
4	2.20	7.30 ± 0.21	9.0 ± 0.6	25.5 ± 3.4	2.15 ± 0.20	51.0	2.0
5	2.18	8.03 ± 0.24	18.1 ± 1.4	75.0 ± 10.5	5.25 ± 0.50	160.0	5.8

Mott and the ES results can be obtained by optimizing the exponential in the hopping probability

$$\gamma_{ij}=\gamma_0\exp(-2r_{ij}/\xi-\varepsilon_{ij}/kT) \quad (4)$$

for an electron to hop a distance r_{ij} between localized states with an energy difference ε_{ij}. Apart from prefactors α_i of order unity [7], Mott's result follows if one assumes that $\varepsilon_{ij}=\alpha_1/gr_{ij}^3$, where g is the constant density of states at the Fermi energy. The ES result is reproduced if one replaces ε_{ij} by $\alpha_2e^2/\kappa r_{ij}$, where e is the electronic charge and κ is the dielectric constant. Although the latter derivation has no rigorous justification, and although there exist alternative ways to derive the former result [7], we emphasize that these two expressions for ε_{ij} basically follow from *dimensional analysis*: $1/gr_{ij}^3$ and $e^2/\kappa r_{ij}$ are the only relevant energy scales for the two limits. Since energies are additive, we next combine the two energies into

$$\varepsilon_{ij}=\alpha_1/gr_{ij}^3+\alpha_2e^2/\kappa r_{ij}\,. \quad (5)$$

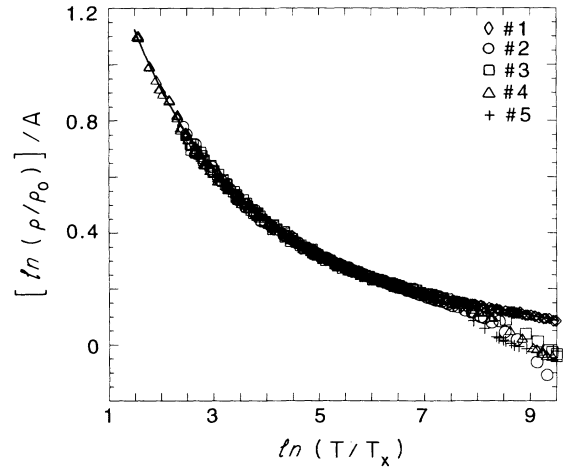

FIG. 2. $[\ln(\rho/\rho_0)]/A$ vs $\ln(T/T_x)$ for five samples of n-type CdSe with different net indium dopant concentrations and different parameters A and T_x. The values of A and T_x, listed in Table I, are determined by fitting the data of Ref. [5] for each sample by Eqs. (1) and (3). The solid line is the function $f(x)$ of Eq. (3). Note the deviations of the data from the collapsed curve at the higher temperatures due to direct thermal activation.

This form is indeed dominated by α_1/gr_{ij}^3 for small r_{ij} and by $\alpha_2e^2/\kappa r_{ij}$ for large r_{ij}, as required [3,4].

Substituting Eq. (5) into Eq. (4), it is now straightforward to maximize γ_{ij} and find the optimal hopping distance

$$(R_h/\xi)^{-2}=(\alpha_2e^2g\xi^2/6\alpha_1\kappa)[(1+T/T_x)^{1/2}-1]\,, \quad (6)$$

with $kT_x=\alpha_2^2e^4g\xi/24\alpha_1\kappa^2$. Substitution into Eqs. (4) and (5), and identification of $1/\rho$ with the optimal γ then yields Eq. (1), with $A=\frac{8}{3}(6\kappa\alpha_1/\alpha_2e^2g\xi^2)^{1/2}$. It is easy to check that $f(x)\approx x^{-1/4}[1+3/2x^{1/2}+O(1/x)]$ for $x\gg1$ and $f(x)\approx3(2x)^{-1/2}[1+x/24+O(x^2)]$ for $x\ll1$. Hence $T_0=A^4T_x=2048\alpha_1/27g\xi^3$ and $T_0'=9A^2\times T_x/2=8\alpha_2e^2/\kappa\xi$. Although α_1 and α_2 may vary among different theories, T_0 and T_0' can be uniquely identified from A and T_x.

Values of A, T_x, and ρ_0 were deduced for each sample from nonlinear least-squares fits of the data by Eqs. (1) and (3). The parameters A and T_x are listed in Table I, as well as values calculated for $T_0=A^4T_x$ and $T_0'=9A^2T_x/2$. The corresponding parameters labeled $(T_0)^I$ and $(T_0')^I$ estimated in earlier work are also listed in the table. We note that A and T_x can be determined much more reliably from experiment than $(T_0)^I$ and $(T_0')^I$: While the former are found from nonlinear fits to all the available data points (excluding only a few at high temperature, where thermal excitation to the conduction band begins to dominate, see below), the latter must use subjective subsets of the data where the asymptotic forms $(T_0/T)^{1/4}$ or $(T_0'/T)^{1/2}$ seem to hold. Thus, fits by Eqs. (1) and (3) for sample 4 using data up to 11 K or up to 6 K yield values for T_0 which agree within 2%, thus providing a rather robust result, in contrast to the earlier determination of T_0' which was rather sensitive to the boundaries of the temperature range used in the fit.

The correction terms for small and large x indicate a much slower deviation from the $x^{-1/2}$ behavior as x increases than from $x^{-1/4}$ in the opposite limit. One thus expects to observe the ES behavior even for $x\gtrsim1$, but the Mott behavior should appear only for very large x. Indeed, Fig. 3 indicates that $f(x)$ is within 10% of the asymptotic behavior $3/(2x)^{1/2}$ (or $1/x^{1/4}$) for $x<4$ (or $x>200$). Thus, the actual crossover occurs gradually for temperatures between $4T_x$ and $200T_x$, with a stronger

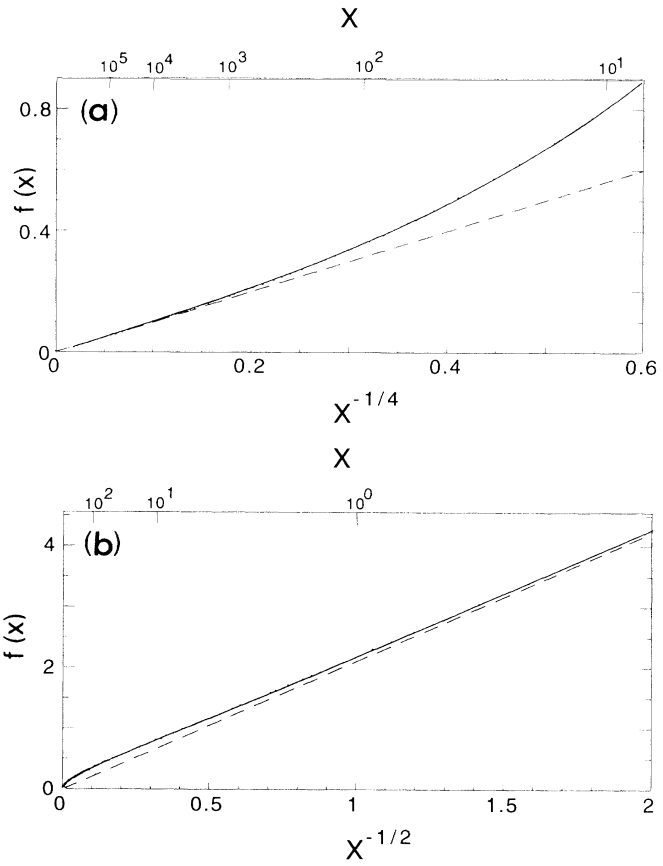

FIG. 3. The function $f(x)$ vs (a) $x^{-1/4}$ and (b) $x^{-1/2}$. The dashed lines denote the asymptotic behavior at high and low x, respectively. Note that $f(x)$ is within 10% of the asymptotic behavior $x^{-1/4}$ for $x > 200$, so that true asymptotic behavior is reached only for very large T. Although the opposite limit at low T is also approached very slowly, the slope is close to its limiting value, $3/2^{1/2}$, over a wide range of x.

variation near the higher bound. This is indeed confirmed by the data of Fig. 1. In practice, this means that one rarely achieves the true asymptotic behavior for high T. Indeed, although our new fits roughly confirm the previously estimated [5] values of T_0', we now find significantly smaller values for T_0. The previous estimates showed an apparently larger slope of $\ln\rho$ vs $T^{-1/4}$ because of the correction (of relative order $3/2x^{1/2}$) as x decreased, as well as because of the sharp decrease of ρ due to direct thermal excitation for very large x. Although the latter effect is not included in our theory, it is easy to identify the data points in Fig. 2 at which it becomes relevant by their significant deviation from the data collapsed curve.

A crossover with decreasing temperature from Mott to ES variable range hopping has been reported in the doped semiconductor CdTe:Cl [8], where the data appear to be similar to CdSe:In. Crossover behavior has also been claimed by Glukhov, Fogel, and Shablo [9] in the granular systems Sn:Ge and Ag:Ge, for which the model proposed does not appear to provide a good fit. As noted by Adkins [10], however, the behavior of the conductivity of these cermets is qualitatively but not quantitatively consistent with ES hopping due to a Coulomb gap. We emphasize that our analysis applies only to simple hopping over an energy barrier, and this may not be the case for the cermets. Alternative models have been proposed, involving, for example, the Coulomb charging energy required to transfer electrons between metal islands, and there is currently no generally accepted explanation for the conductivity of these granular metals [10].

We note again that our dimensional analysis does not depend on any details of the many-body Coulomb system. Our results could also be obtained by optimizing Eq. (4) with respect to ε_{ij} instead of r_{ij}, using $r_{ij} \propto 1/(g\varepsilon_{ij})^{1/3}$ and replacing $g(\varepsilon)$ by a smooth function which crosses over from behaving as ε^2 (for small ε) to a constant (for large ε), as implied in Refs. [3,4]. Alternatively, one could use a percolation model in the four-dimensional $r-E$ space [7], with one-particle excitations which obey the ES constraint $\varepsilon - \alpha_2 e^2/\kappa r > 0$. We expect all these calculations to yield crossover functions very similar to our Eq. (3). In any case, we hope that the remarkably good fit shown in Fig. 2 will stimulate both experimentalists to try fitting Eq. (3) to other systems (including those that seem to be in the asymptotic Mott regime) and theorists to search for more rigorous derivations.

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